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OPTIMAL STIFFLY STABLE METHODS FOR ORDINARY DIFFERENTIAL EQUATIONS

by

M. K. Jain
V. K. Srivastava

June 1970

DEPARTMENT OF COMPUTER SCIENCE
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN · URBANA, ILLINOIS

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E R R A T A   T O

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$$+ \frac{171}{726} y_{n-4} + \frac{13}{726} y_{n-5} - \frac{9}{726} y_{n-6} + h \frac{300}{726} y'_{n-1}$$

ACKNOWLEDGMENT

We wish to thank Professor C. W. Gear for his helpful suggestions. Thanks are also extended to Miss Barbara Hurdle for typing of the final manuscript.

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ABSTRACT

The purpose of this report is to discuss one parameter methods for the numerical integration of stiff differential equations, i.e., systems with widely separated time constants. The methods which are optimal in terms of least amount of solution history data to be saved at each step of the corrector iteration have been known for order as high as six. We find that in one parameter methods the stability and accuracy are controlled by the same variable γ. Suitable values of γ lead to methods which have either optimal accuracy or optimal stability. The methods of order six have been presented. The section of the locus $\rho(\xi)/\sigma(\xi)$ for methods of order six is shown in Figure 7.

LIST OF FIGURES

1. INTRODUCTION

Many numerical problems in applied mathematics entail the solution of systems of ordinary differential equations with a property given by the following definition.

<u>Definition.</u> *A system of ordinary differential equations* $\vec{y}\,' = \vec{f}(t, \vec{y})$, $\vec{y}(a) = \vec{\eta}$ *is said to be stiff if the eigen values of the matrix* $(\frac{\partial f}{\partial y})$ *has at every point t negative real parts, and differ greatly in magnitude.*

Equations of this form frequently arise in physical equilibrium problems such as chemical or nuclear reactions where there are many components with a large range of time constants. The standard numerical integration methods are unstable if the step size used is much greater than the smallest time constant. Dahlquist [1] has introduced the concept of A-stability. The theorem of Dahlquist states that among all linear multistep methods the trapezoidal rule is the most accurate. Gear [2,3] has developed stiffly stable methods based on the necessary requirements of the stiff differential equations. He has obtained stiffly stable methods of order as high as six. Dill [4] has extended this analysis to the methods of order seven and eight. Jain and Srivastava [5] examined a class of methods and obtained stiffly stable methods of order eleven. The purpose of this report is to obtain optimal stiffly stable methods for the stiff differential equation

(1) $$\frac{dy}{dt} = f(t, y), \; y(a) = \eta$$

2. OPTIMAL STIFFLY STABLE METHODS

The requirements for the stiffly stable methods are shown in Figure 1.

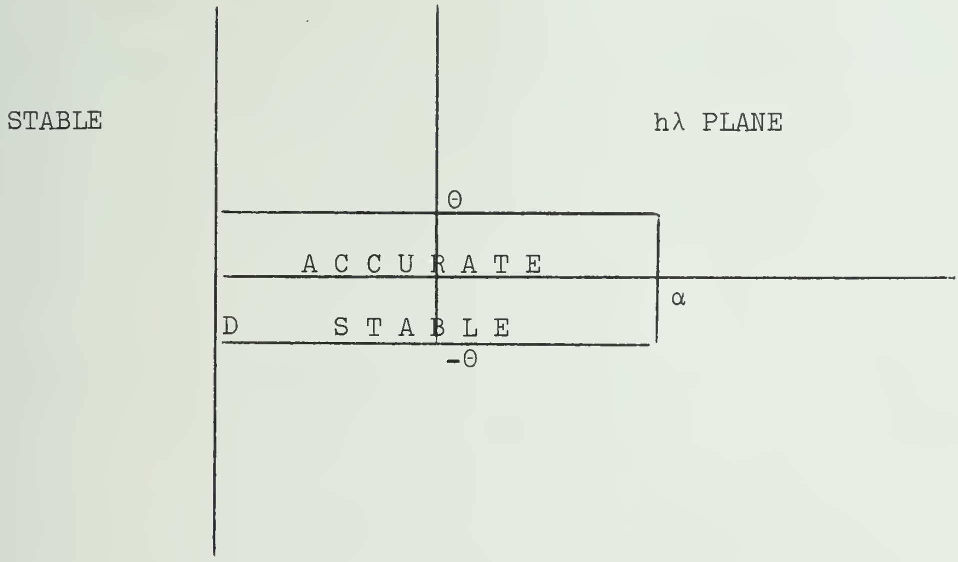

Figure 1

STABILITY AND ACCURACY REGIONS

The existence of stiffly stable methods depends on the parameters D, Θ, α and on the definition of accuracy. The usual definition of accuracy is that of the order. Dahlquist has shown that if D is zero then the order of the method cannot exceed two. Here we have obtained stiffly stable methods with extended region of stability of order as high as six for suitable parameters D, Θ, and α.

<u>Third Order Formula</u>: Multistep formulas may be obtained by writing a linear relation between values of the function and derivative at specified points and determining the coefficients in the relation by expansions in Taylor series about an arbitrary point. For instance, we may write

(2) $$y_{n+1} = \alpha_1 y_n + \alpha_2 y_{n-1} + \alpha_3 y_{n-2} + \alpha_4 y_{n-3} + h\beta_0 y'_{n+1} + T_n$$

The fourth order formula, that is, the one whose truncation error is of order h^5, has been obtained by Gear

(3) $$y_{n+1} = \frac{48}{25} y_n - \frac{36}{25} y_{n-1} + \frac{16}{25} y_{n-2} - \frac{3}{25} y_{n-3} + h \frac{12}{25} y'_{n+1} - \frac{12}{125} h^5 y_n^{(5)}$$

If instead of requiring that T_n, the truncation error, should be of fifth order, we specify a fourth order truncation error we find that there is a one-parameter family of methods.

This may be written

(4) $$y_{n+1} = \left(\frac{48}{25} - \frac{26}{300}\gamma\right) y_n - \left(\frac{36}{25} - \frac{57}{300}\gamma\right) y_{n-1} + \left(\frac{16}{25} - \frac{42}{300}\gamma\right) y_{n-2} - \left(\frac{3}{25} - \frac{11}{300}\gamma\right) y_{n-3} + h\left(\frac{12}{25} + \frac{6}{300}\gamma\right) y'_{n+1} + T_n$$

or alternatively

$$y_{n+1} = \frac{48}{25} y_n - \frac{36}{25} y_{n-1} + \frac{16}{25} y_{n-2} - \frac{3}{25} y_{n-3} + h \frac{12}{25} y'_{n+1} - \frac{\gamma}{300} \left[26y_n - 57y_{n-1} + 42y_{n-2} - 11y_{n-3} - h6y'_{n+1}\right] + T_n$$

where

$$T_n = \begin{cases} -\gamma h^4 y_n^{(4)}/24 & (\gamma \neq 0) \\ -12h^5 y_n^{(5)}/125 & (\gamma = 0) \end{cases}$$

This later way of writing emphasizes the nature of the integration formula. It is seen to be composed of the fourth order formula with the minus of a third order restrictive condition. Note also that $\gamma = \frac{36}{11}$ gives the third order stiffly stable method

$$y_{n+1} = \frac{18}{11} y_n - \frac{9}{11} y_{n-1} + \frac{2}{11} y_{n-2} + h \frac{6}{11} y'_{n+1} - \frac{3}{22} h^4 y_n^{(4)}$$

The discretization error of the formula (4) is defined as the difference between the value y_n calculated from (4) and the exact solution $y(x_n)$.

Define $\quad \varepsilon_n = y_n - y(x_n)$

Then the error ε_n obeys the difference equation

(5) $$\varepsilon_{n+1} = \left(\frac{48}{25} - \frac{26}{300}\gamma\right)\varepsilon_n - \left(\frac{36}{25} - \frac{57}{300}\gamma\right)\varepsilon_{n-1} + \left(\frac{16}{25} - \frac{42}{300}\gamma\right)\varepsilon_{n-2}$$
$$- \left(\frac{3}{25} - \frac{11}{300}\gamma\right)\varepsilon_{n-3} + h\lambda\left(\frac{12}{25} + \frac{6}{300}\gamma\right)\varepsilon_{n+1} - T_n$$

for the differential equation $y' = \lambda y$.

This linear difference equation with constant coefficients may be solved by setting $\varepsilon_n = \xi^n$, which gives the characteristic equation

(6) $$\rho(\xi) - h\lambda\, \sigma(\xi) + T_n = 0$$

where

$$\rho(\xi) = \xi^4 - \left(\frac{48}{25} - \frac{26}{300}\gamma\right)\xi^3 + \left(\frac{36}{25} - \frac{57}{300}\gamma\right)\xi^2 - \left(\frac{16}{25} - \frac{42}{300}\gamma\right)\xi$$
$$+ \left(\frac{3}{25} - \frac{11}{300}\gamma\right)$$

and

$$\sigma(\xi) = \left(\frac{12}{25} + \frac{6}{300}\gamma\right)\xi^4$$

It is necessary to bound the solution of the inhomogeneous difference equation (5), Henrici [6]. It depends on the stability of the corresponding homogeneous equation which is obtained when T_n is set to zero. The difference equation is stable if and only if all roots of the polynomial equation

(7) $$\rho(\xi) - h\lambda\,\sigma(\xi) = 0$$

are inside the unit circle or on the unit circle and simple. If stiff differential equations are to be integrated with large values of h, then large values of $h\lambda$ must not make (7) unstable. Letting $h\lambda \to \infty$, the roots of (7) approach those of $\sigma(\xi) = 0$. This implies that the polynomial $\sigma(\xi)$ must not have roots outside the unit circle and those roots ξ_i for which $|\xi_i| = 1$ are simple. This condition is already satisfied by $\sigma(\xi)$ in this case. For stiff stability we want $h\lambda$ values such that (7) has roots inside the unit circle or on the unit circle and simple. This region is bounded by the locus of $\rho(\xi)/\sigma(\xi)$ in the $h\lambda$-plane for $\xi = e^{i\Theta}$, $\Theta\varepsilon[0, 2\pi]$. For different values of γ the locus of $\rho(\xi)/\sigma(\xi)$ is shown in Figure 2.

The locus boundaries are closed and symmetrical about the real axis, pass through the origin and steadily decrease in area as γ increases from 0 to 7, approximately. At $\gamma = 7$, the formula ceases to be stiffly stable. The intercept of the boundary on the real axis is given by

(8) $$h\lambda = \frac{4}{3}\,\frac{192 - 17\gamma}{24 + \gamma}$$

$\gamma = \frac{36}{11}$ gives third order formula which is optimal in terms of least amount of solution history data to be saved at each step of the corrector iteration.

Here we find that the values of γ in the interval $0 < \gamma < \frac{36}{11}$ give third order formulas which are stiffly stable with reduced truncation error coefficient. We shall denote such formulas by P. Similarly for the values of γ in the interval $\frac{36}{11} < \gamma < 7$, we obtain third order stiffly stable formulas which have extended region of stability. We shall denote such formulas by Q. The locus of $\rho(\xi)/\sigma(\xi)$, $\xi = e^{i\theta}$, $\theta\epsilon[0, 2\pi]$ for $\gamma = 6$ is shown in Figure 3. The P and Q type formulas for $\gamma = 2$ and $\gamma = 6$ are listed here. The values of parameters C (error constant), D, Θ and $\max|\xi|$ (ξ_i being the roots of $\rho(\xi) = 0$) for formulas of order $p \leq 6$ are listed in the table.

(P)
$$y_{n+1} = \frac{262}{150} y_n - \frac{159}{150} y_{n-1} + \frac{54}{150} y_{n-2} - \frac{7}{150} y_{n-3} + h \frac{78}{150} y'_{n+1} - \frac{1}{12} h^4 y_n^{(4)}$$

(Q)
$$y_{n+1} = \frac{14}{10} y_n - \frac{3}{10} y_{n-1} - \frac{2}{10} y_{n-2} + \frac{1}{10} y_{n-3} + h \frac{6}{10} y'_{n+1} - \frac{1}{4} h^4 y_n^{(4)}$$

One parameter family of formulas together with P and Q type formulas for order six are given here.

<u>Fourth Order Formula</u>: One parameter family of fourth order formula is given by

(9)
$$y_{n+1} = \frac{300}{137} y_n - \frac{300}{137} y_{n-1} + \frac{200}{137} y_{n-2} - \frac{75}{137} y_{n-3} + \frac{12}{137} y_{n-4} + h \frac{60}{137} y'_{n+1} - \frac{\gamma}{3288} [77y_n - 214y_{n-1} + 234y_{n-2} - 122y_{n-3} + 25y_{n-4} - h\, 12y'_{n+1}] - \frac{\gamma}{120} h^5 y_n^{(5)}$$

The characteristic equation is

$$\xi^5 - \frac{1}{137}(300 - \frac{77}{24}\gamma)\xi^4 + \frac{1}{137}(300 - \frac{214}{24}\gamma)\xi^3 - \frac{1}{137}(200 - \frac{234}{24}\gamma)\xi^2 + \frac{1}{137}(75 - \frac{122}{24}\gamma)\xi - \frac{1}{137}(12 - \frac{25}{12}\gamma) - h\lambda\frac{1}{137}(60 + \frac{12}{24}\gamma)\xi^5 = 0 \tag{10}$$

The locus of $\rho(\xi)/\sigma(\xi)$ for different values of γ is shown in Figure 4. $\gamma = \frac{288}{25}$ gives fourth order formula obtained by Gear. $\gamma \geq 25$ does not give stiffly stable methods. The formulas for $\gamma = 5$ and $\gamma = 24$ are listed below.

$$y_{n+1} = \frac{6815}{3288}y_n - \frac{6130}{3288}y_{n-1} + \frac{3630}{3288}y_{n-2} - \frac{1190}{3288}y_{n-3} + \frac{163}{3288}y_{n-4} + h\frac{1500}{3288}y'_{n+1} - \frac{1}{24}h^5y_n^{(5)} \tag{P}$$

$$y_{n+1} = \frac{223}{137}y_n - \frac{86}{137}y_{n-1} - \frac{34}{137}y_{n-2} + \frac{47}{137}y_{n-3} - \frac{13}{137}y_{n-4} + h\frac{72}{137}y'_{n+1} - \frac{1}{5}h^5y_n^{(5)} \tag{Q}$$

<u>Fifth Order Formula</u>: One parameter family of fifth order formula is

$$\begin{aligned} y_{n+1} = {} & \frac{1}{147}(360 - \frac{522}{720}\gamma)y_n - \frac{1}{147}(450 - \frac{1755}{720}\gamma)y_{n-1} \\ & + \frac{1}{147}(400 - \frac{2540}{720}\gamma)y_{n-2} - \frac{1}{147}(225 - \frac{1980}{720}\gamma)y_{n-3} \\ & + \frac{1}{147}(72 - \frac{810}{720}\gamma)y_{n-4} - \frac{1}{147}(10 - \frac{137}{720}\gamma)y_{n-5} \\ & + h\frac{1}{147}(60 + \frac{60}{720}\gamma)y'_{n+1} - \gamma\frac{h^6y_n^{(6)}}{720} \end{aligned} \tag{11}$$

The locus of $\rho(\xi)/\sigma(\xi)$ for different values of γ is given in Figure 5. $\gamma = \frac{7200}{137}$ gives fifth order stiffly stable formula and has the virtue of economy of storage. For $\gamma > 110$, fifth order stiffly stable formula ceases to exist. The stiffly stable formulas for $\gamma = 36$ and $\gamma = 96$ becomes

(P)
$$y_{n+1} = \frac{6678}{2940} y_n - \frac{7245}{2940} y_{n-1} + \frac{5460}{2940} y_{n-2} - \frac{2520}{2940} y_{n-3}$$
$$+ \frac{630}{2940} y_{n-4} - \frac{63}{2940} y_{n-5} + h \frac{1260}{2940} y'_{n+1} - \frac{1}{20} h^6 y_n^{(6)}$$

(Q)
$$y_{n+1} = \frac{4356}{2205} y_n - \frac{3240}{2205} y_{n-1} + \frac{920}{2205} y_{n-2} + \frac{585}{2205} y_{n-3}$$
$$- \frac{540}{2205} y_{n-4} + \frac{124}{2205} y_{n-5} + h \frac{1020}{2205} y'_{n+1} - \frac{2}{15} h^6 y_n^{(6)}$$

<u>Sixth Order Formula:</u>

(12)
$$y_{n+1} = \frac{1}{1089} (2940 - \frac{669}{720}\gamma) y_n - \frac{1}{1089} (4410 - \frac{2637}{720}\gamma) y_{n-1}$$
$$+ \frac{1}{1089} (4900 - \frac{4745}{720}\gamma) y_{n-2} - \frac{1}{1089} (3675 - \frac{4920}{720}\gamma) y_{n-3}$$
$$+ \frac{1}{1089} (1764 - \frac{3015}{720}\gamma) y_{n-4} - \frac{1}{1089} (490 - \frac{1019}{720}\gamma) y_{n-5}$$
$$+ \frac{1}{1089} (60 - \frac{147}{720}\gamma) y_{n-6} + h \frac{1}{1089} (420 + \frac{60}{720}\gamma) y'_{n+1}$$
$$- \frac{\gamma}{5040} h^7 y_n^{(7)}$$

$\gamma = \frac{43200}{147}$ gives six order stiffly stable formula as obtained by Gear. $\gamma = 0$ gives a seventh order formula which is unstable. The locus of $\rho(\xi)/\sigma(\xi)$ as a function of γ is shown in Figure 6. The stiffly stable formulas for $\gamma = 240$ and $\gamma = 360$ are listed here. The formula is stiffly stable in the interval $15 < \gamma < 620$, approximately.

(P)
$$y_{n+1} = \frac{8151}{3267} y_n - \frac{10593}{3267} y_{n-1} + \frac{9955}{3267} y_{n-2} - \frac{6105}{3267} y_{n-3}$$
$$+ \frac{2277}{3267} y_{n-4} - \frac{451}{3267} y_{n-5} + \frac{33}{3267} y_{n-6} + h \frac{1320}{3267} y'_{n+1}$$
$$- \frac{1}{21} h^7 y_n^{(7)}$$

(Q)
$$y_{n+1} = \frac{1737}{726} y_n - \frac{2061}{726} y_{n-1} + \frac{1685}{726} y_{n-2} - \frac{810}{726} y_{n-3}$$
$$+ \frac{171}{726} y_{n-4} - \frac{13}{726} y_{n-5} - \frac{9}{726} y_{n-6} + h \frac{300}{726} y'_{n+1}$$
$$- \frac{1}{14} h^7 y_n^{(7)}$$

TABLE OF VALUES OF THE PARAMETERS

Order and Type of the Method		γ	D	Θ	$\max_{\xi\neq 1}\lvert\xi\rvert$	C
3	P	2	-0.1777	84°14'	0.43635	-25/156
	Q	6	-0.0535	86°50'	0.49	-5/12
4	P	5	-1.3953	69°20'	0.62757	-137/1500
	Q	24	-0.4238	77°26'	0.60328	-137/360
5	P	36	-3.2166	59°12'	0.743	-147/1260
	Q	96	-1.4966	66°3'	0.71381	-147/510
6	P	240	-7.1812	48°36'	0.88444	-363/3080
	Q	360	-5.0149	50°34'	0.84820	-121/700

3. CONCLUSIONS

The stiffly stable methods have been found very efficient in integrating stiff differential equations because they allow a much larger step size while maintaining stability. Here we have developed one parameter family of methods suited to integrating stiff differential equations. It is found that stability and accuracy are controlled by the same variable γ. The methods which are optimal in terms of least amount of solution history data to be saved at each step were obtained by Gear for order as high as six. A suitable value of γ leads to methods which have optimal accuracy or optimal stability without violating the condition of economy of storages. There is a great advantage to be gained by the use of a formula with optimal stability when solving sets of simultaneous differential equations whose solution approximate to exponentials with real negative arguments. An optimal stability enables the interval of integration to be increased without causing instability. However, in general the value of γ will vary with the behavior of the equations we are attempting to solve. Parametric methods for the solution of ordinary differential equations have also been discussed by Hamming [7] and Robertson [8]. Applications of these and similar formulas to predictor-corrector methods will be discussed separately.

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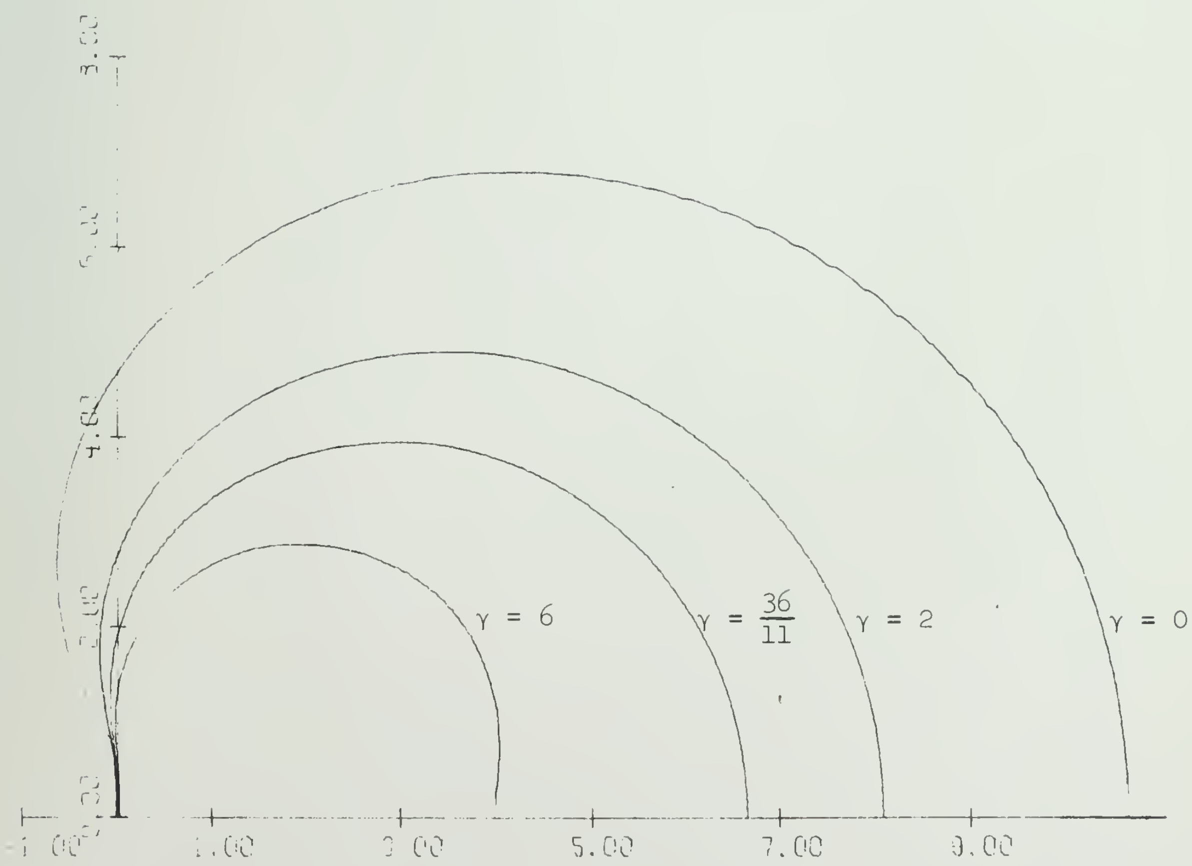

Figure 2
Third Order Formula
STIFFLY STABLE REGION AS A FUNCTION OF γ

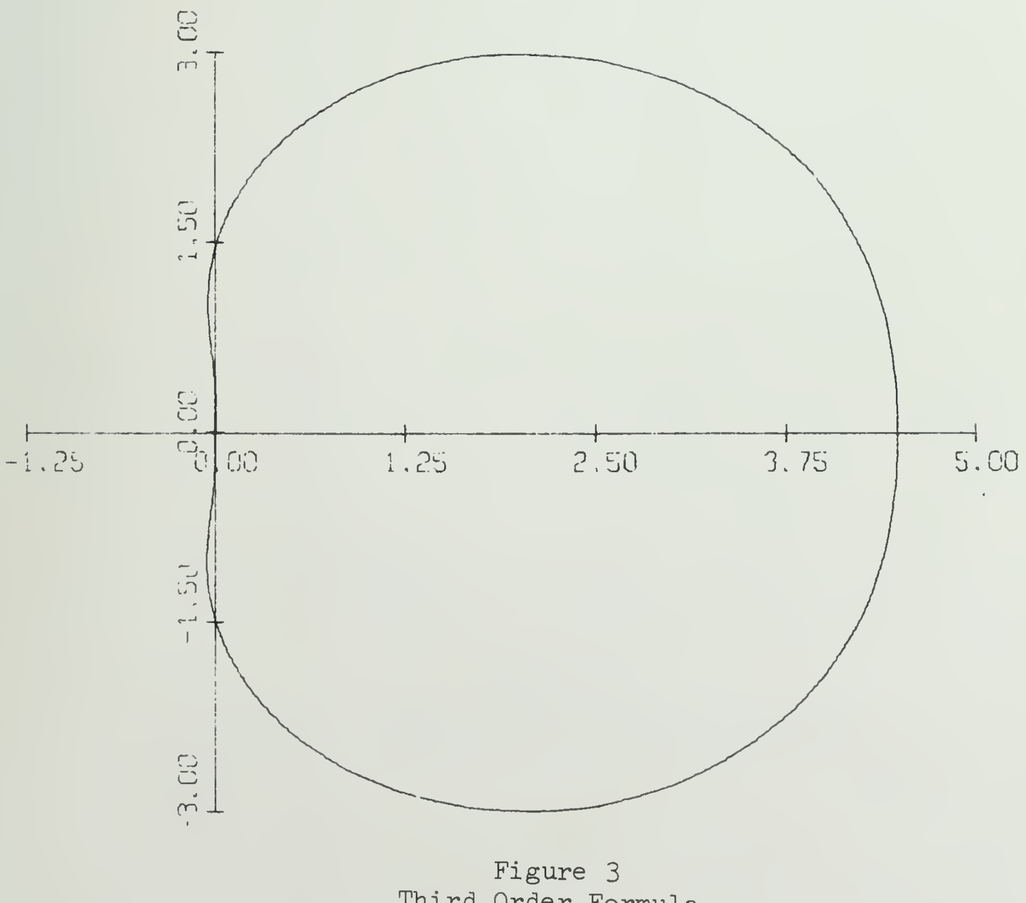

Figure 3
Third Order Formula
LOCUS OF $\rho(\xi)/\sigma(\xi)$, $\xi = e^{i\theta}$, $\theta \varepsilon [0, 2\pi]$

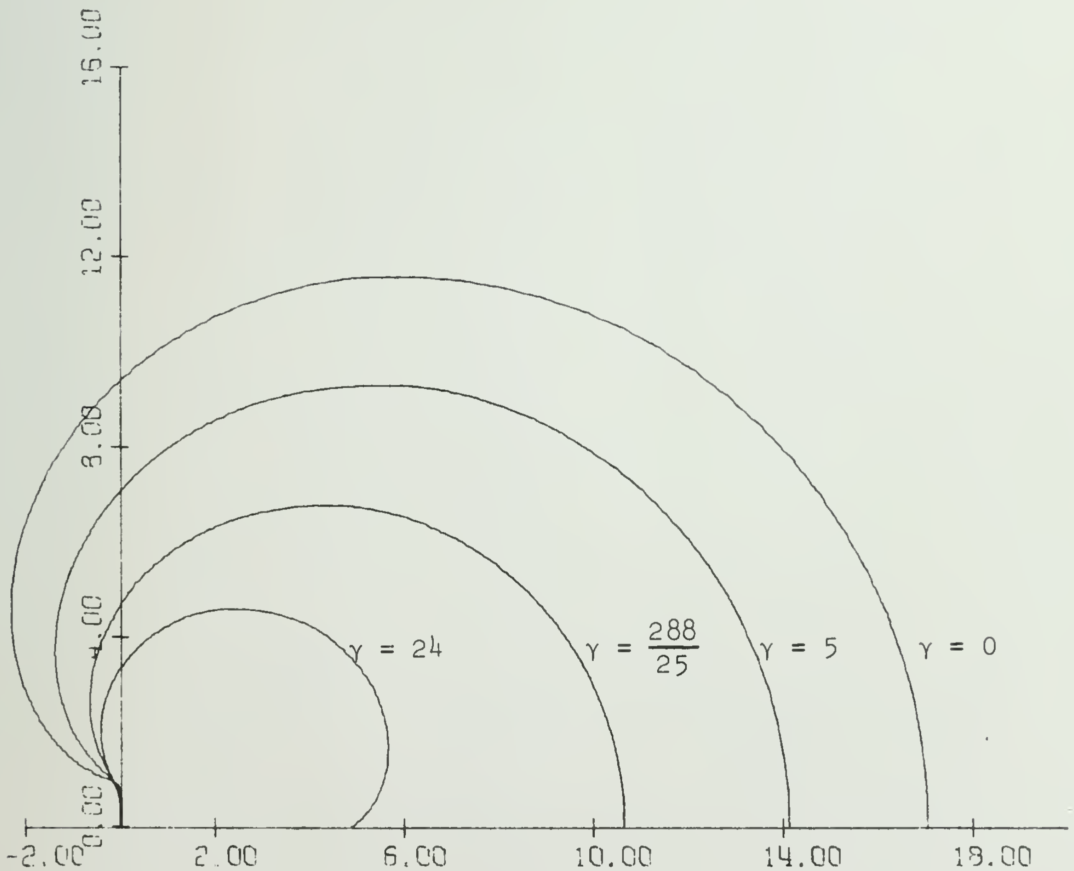

Figure 4
Fourth Order Formula
STIFFLY STABLE REGION AS A FUNCTION OF γ

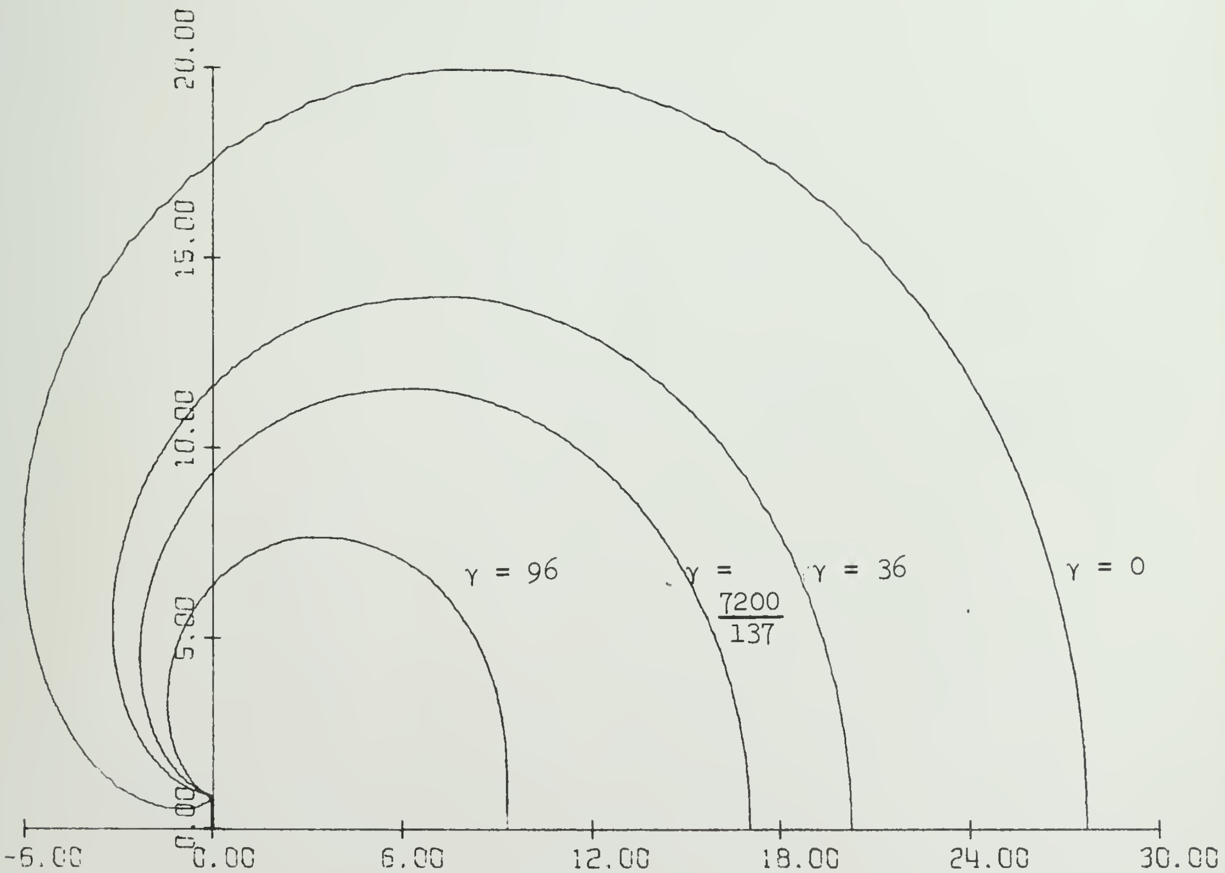

Figure 5
Fifth Order Formula
STIFFLY STABLE REGION AS A FUNCTION OF γ

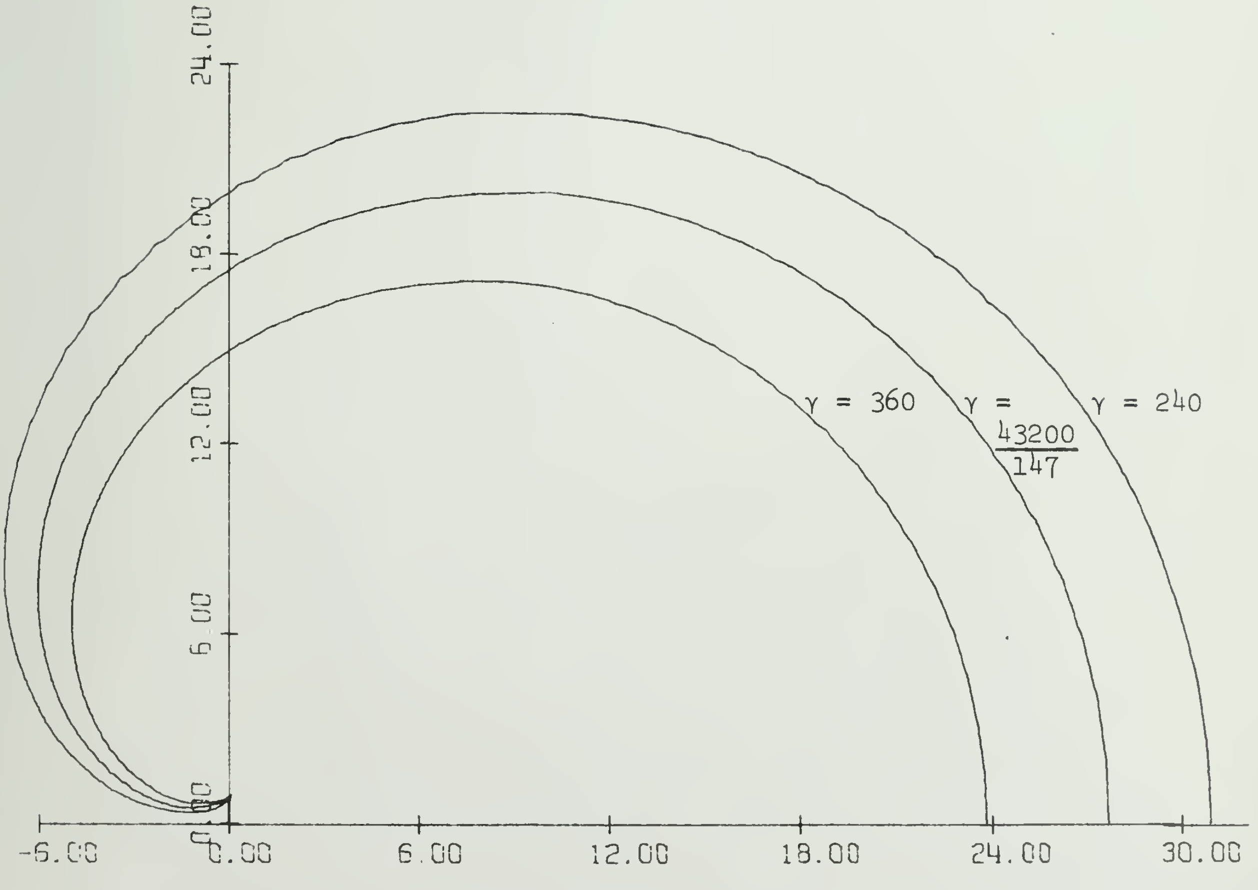

Figure 6
Sixth Order Formula
STIFFLY STABLE REGION AS A FUNCTION OF γ

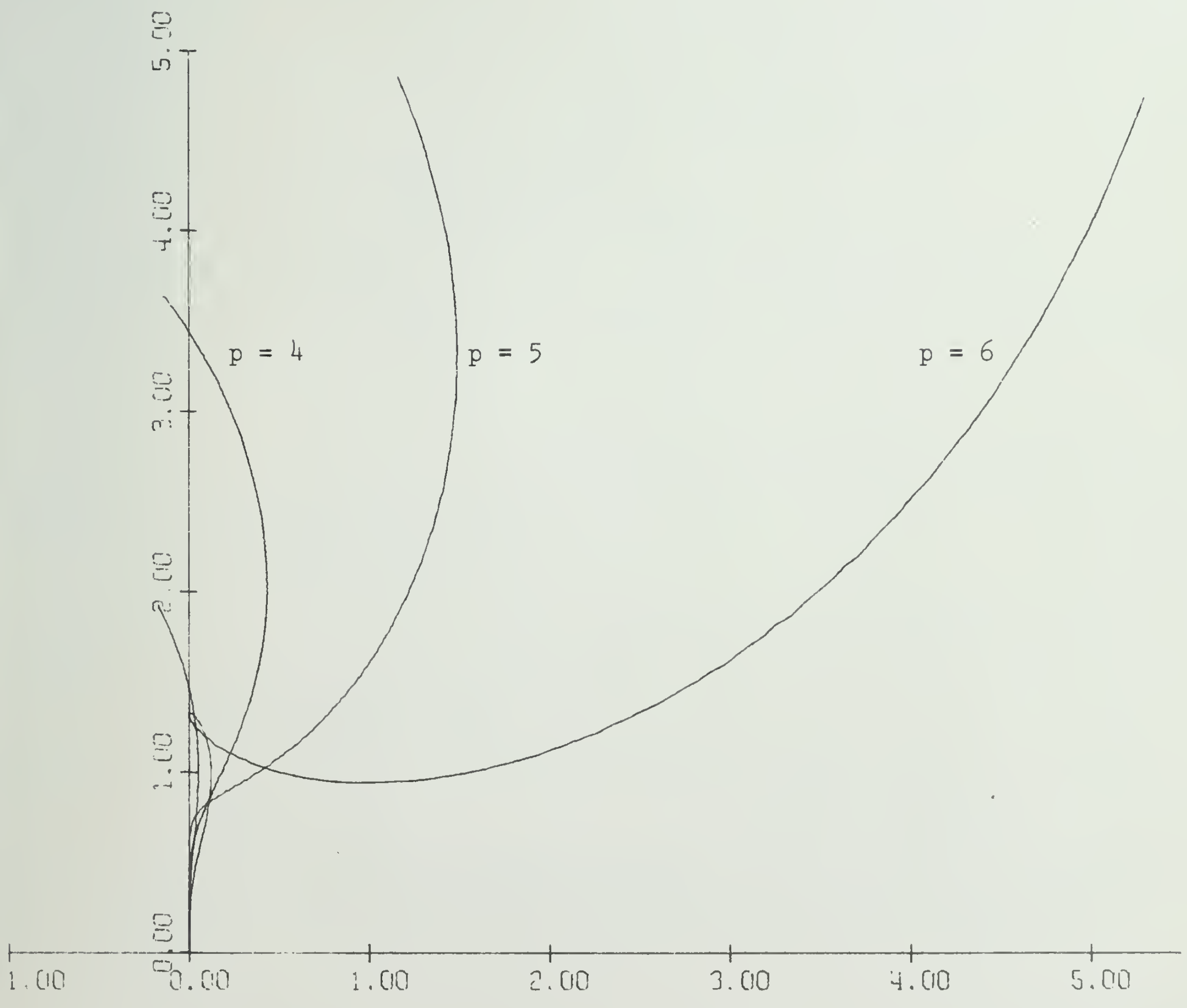

Figure 7
SECTION OF LOCUS OF $\rho(\xi)/\sigma(\xi)$ FOR $p \leq 6$

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